wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2023 – 08:29 PM EDT

PDB ID	:	2PVY
Title	:	Crystal Structure of FGF Receptor 2 (FGFR2) Kinase Domain Harboring the Pathogenic K659N Mutation Responsible for an Unclassified Craniosynostosis Syndrome.
Authors	:	Chen, H.; Mohammadi, M.
Deposited on	:	2007-05-10
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

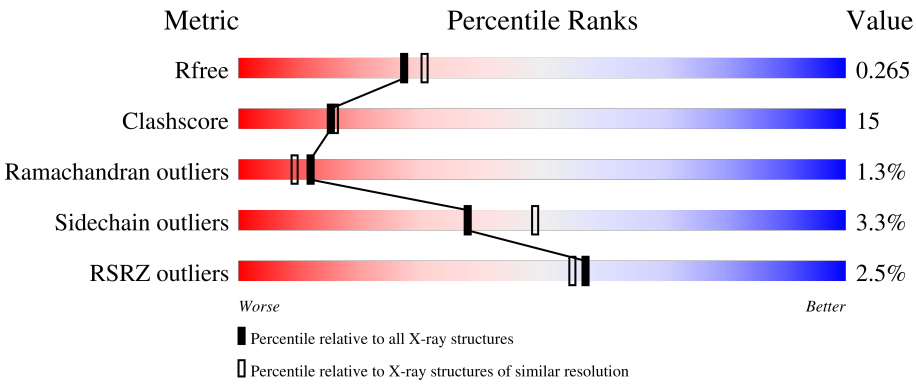
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	324	2% 65% 22% • 11%
1	B	324	2% 62% 23% • 12%
1	C	324	3% 66% 21% • 12%
1	D	324	2% 62% 23% • • 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9429 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2280	1449	390	421	20	0	0	0
1	B	286	2278	1452	389	417	20	0	0	0
1	C	285	2270	1448	385	416	21	0	0	0
1	D	283	2246	1431	382	413	20	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	expression tag	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression tag	UNP P21802
A	452	HIS	-	expression tag	UNP P21802
A	453	HIS	-	expression tag	UNP P21802
A	454	HIS	-	expression tag	UNP P21802
A	455	SER	-	expression tag	UNP P21802
A	456	GLN	-	expression tag	UNP P21802
A	457	ASP	-	expression tag	UNP P21802
A	491	ALA	CYS	engineered mutation	UNP P21802
A	659	ASN	LYS	engineered mutation	UNP P21802
B	445	MET	-	expression tag	UNP P21802
B	446	GLY	-	expression tag	UNP P21802
B	447	SER	-	expression tag	UNP P21802
B	448	SER	-	expression tag	UNP P21802
B	449	HIS	-	expression tag	UNP P21802
B	450	HIS	-	expression tag	UNP P21802

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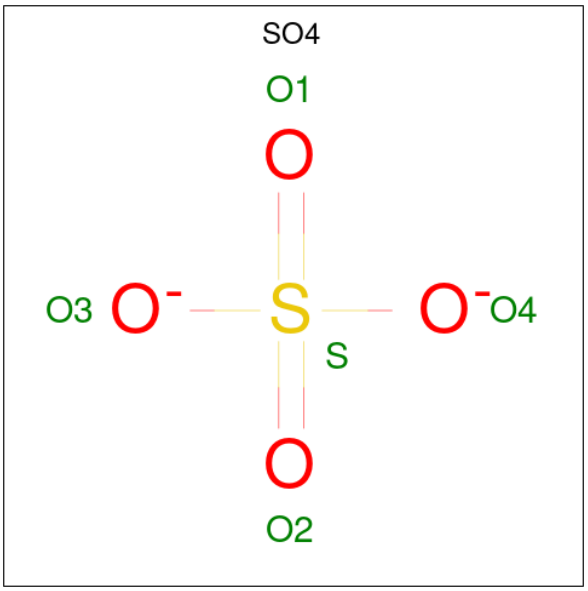
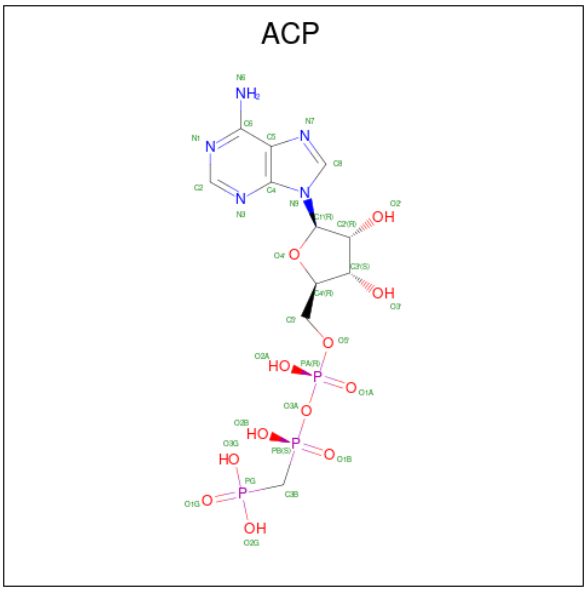
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	expression tag	UNP P21802
B	452	HIS	-	expression tag	UNP P21802
B	453	HIS	-	expression tag	UNP P21802
B	454	HIS	-	expression tag	UNP P21802
B	455	SER	-	expression tag	UNP P21802
B	456	GLN	-	expression tag	UNP P21802
B	457	ASP	-	expression tag	UNP P21802
B	491	ALA	CYS	engineered mutation	UNP P21802
B	659	ASN	LYS	engineered mutation	UNP P21802
C	445	MET	-	expression tag	UNP P21802
C	446	GLY	-	expression tag	UNP P21802
C	447	SER	-	expression tag	UNP P21802
C	448	SER	-	expression tag	UNP P21802
C	449	HIS	-	expression tag	UNP P21802
C	450	HIS	-	expression tag	UNP P21802
C	451	HIS	-	expression tag	UNP P21802
C	452	HIS	-	expression tag	UNP P21802
C	453	HIS	-	expression tag	UNP P21802
C	454	HIS	-	expression tag	UNP P21802
C	455	SER	-	expression tag	UNP P21802
C	456	GLN	-	expression tag	UNP P21802
C	457	ASP	-	expression tag	UNP P21802
C	491	ALA	CYS	engineered mutation	UNP P21802
C	659	ASN	LYS	engineered mutation	UNP P21802
D	445	MET	-	expression tag	UNP P21802
D	446	GLY	-	expression tag	UNP P21802
D	447	SER	-	expression tag	UNP P21802
D	448	SER	-	expression tag	UNP P21802
D	449	HIS	-	expression tag	UNP P21802
D	450	HIS	-	expression tag	UNP P21802
D	451	HIS	-	expression tag	UNP P21802
D	452	HIS	-	expression tag	UNP P21802
D	453	HIS	-	expression tag	UNP P21802
D	454	HIS	-	expression tag	UNP P21802
D	455	SER	-	expression tag	UNP P21802
D	456	GLN	-	expression tag	UNP P21802
D	457	ASP	-	expression tag	UNP P21802
D	491	ALA	CYS	engineered mutation	UNP P21802
D	659	ASN	LYS	engineered mutation	UNP P21802

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O P 31 11 5 12 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	74	Total O 74 74	0	0
4	B	51	Total O 51 51	0	0
4	C	44	Total O 44 44	0	0
4	D	84	Total O 84 84	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fibroblast growth factor receptor 2

Chain A: 2% 65% 22% • 11%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER GLN ASP PRO MET LEU ALA GLY VAL SER GLU TYR E467 L468 P477 R478 D479 K485 P486 L487 GLY GLU GLY ALA PHE GLY Q494 V495 V496 G502 I503 D504 K505 D506 K507 P508 E525 K526 D527 L528 V532 M537 M540

I541 I548 N549 T555 Q556 D557 E565 N571 L572 R573 E574 Y575 R579 G583 M584 GLU TYR SER TYR D589 I590 P594 E595 E596 Q597 M598 I599 F600 V604 S605 C606 Q609 L610 E615 Y616 L617 K621 C622 R625 R630 L633 V634 T635 E636 N637

M640 K641 L647 N652 N653 K658 N659 T660 T661 P666 E673 R678 V679 L692 P708 V709 E710 E711 D723 N727 C728 T729 F750 K751 V754 E755 R759 I760 L761 T762 L763 T764 THR ASN GLU GLU

• Molecule 1: Fibroblast growth factor receptor 2

Chain B: 2% 62% 23% • 12%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER GLN ASP PRO MET LEU ALA G462 V463 S464 E465 Y466 E467 P476 D479 L487 GLY GLU GLY ALA PHE GLY Q494 V495 I503 D506 K507 P508 V512 V516 L519 L528 M535 E536 M537 M540 I541 K545

N546 I547 I548 N549 A553 L560 Y561 V562 K569 G570 N571 L572 R573 E574 Y575 R579 G583 MET GLU TYR SER TYR D589 I590 F600 S605 Q609 L610 E615 Y616 L617 C622 R625 R630 N631 V632 L633 V634 N638 V639 L647 D650 I651 N652 N653

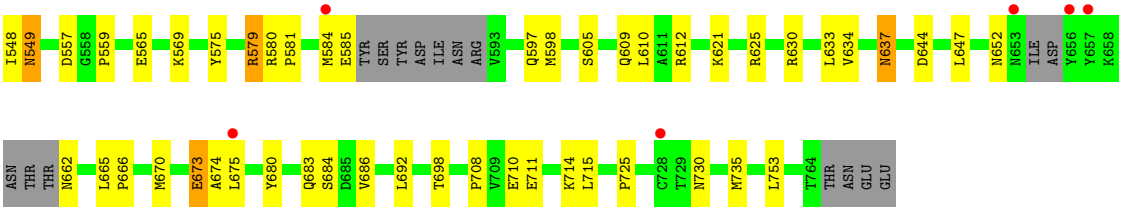
ILE ASP Y656 Y657 K658 ASN THR THR ASN G663 R664 L665 P666 V667 K668 W669 M670 A671 P672 E673 A674 L675 F676 D677 R678 V679 Y680 S684 W687 L692 M693 P708 E711 L712 F713 K714 E718 D723 N727 C728 T729 M735 M736 W740 K751 Q752 L753 D756

L757 D758 R759 T764 THR ASN GLU GLU

• Molecule 1: Fibroblast growth factor receptor 2

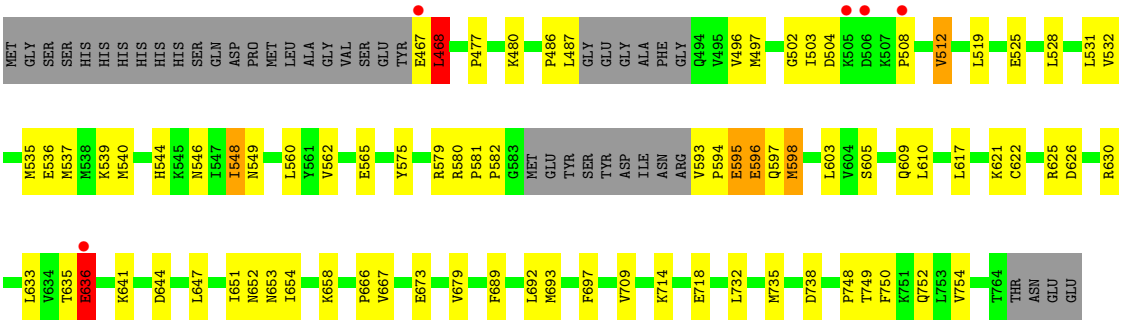
Chain C: 3% 66% 21% • 12%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER GLN ASP PRO MET LEU ALA G462 V463 S464 E465 Y466 E467 L468 K485 P486 L487 GLY GLU GLY ALA PHE GLY Q494 V495 V496 M497 A500 I503 D504 K505 D506 K507 P508 K509 E510 A511 V512 L519 E525 L528 K545



- Molecule 1: Fibroblast growth factor receptor 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.58Å 70.47Å 85.69Å 92.19° 112.31° 116.19°	Depositor
Resolution (Å)	25.00 – 2.20 42.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.20) 96.0 (42.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	9.49 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.276 0.225 , 0.265	Depositor DCC
R_{free} test set	3336 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.058 for k,h,-h-k-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9429	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ACP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.37	0/2327	0.64	0/3151
1	B	0.36	0/2324	0.60	0/3138
1	C	0.35	0/2316	0.58	0/3127
1	D	0.37	0/2293	0.62	0/3104
All	All	0.36	0/9260	0.61	0/12520

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2280	0	2257	70	0
1	B	2278	0	2275	75	0
1	C	2270	0	2269	71	0
1	D	2246	0	2239	73	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	17	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	14	0	0
3	C	17	0	9	0	0
3	D	17	0	9	0	0
4	A	74	0	0	3	0
4	B	51	0	0	1	0
4	C	44	0	0	0	0
4	D	84	0	0	1	0
All	All	9429	0	9081	273	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 273 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:MET:HE2	1:B:753:LEU:HD22	1.48	0.94
1:B:463:VAL:HG13	1:B:528:LEU:HD23	1.50	0.94
1:A:595:GLU:HG3	1:D:636:GLU:HB3	1.50	0.94
1:C:580:ARG:HD3	1:C:584:MET:HG2	1.51	0.90
1:A:549:ASN:H	1:A:549:ASN:HD22	0.95	0.89

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	282/324 (87%)	264 (94%)	14 (5%)	4 (1%)	11 8
1	B	276/324 (85%)	262 (95%)	11 (4%)	3 (1%)	14 12
1	C	275/324 (85%)	257 (94%)	15 (6%)	3 (1%)	14 12
1	D	277/324 (86%)	263 (95%)	10 (4%)	4 (1%)	11 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1110/1296 (86%)	1046 (94%)	50 (4%)	14 (1%)	12 9

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	ILE
1	A	636	GLU
1	A	763	LEU
1	D	468	LEU
1	D	596	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	246/284 (87%)	238 (97%)	8 (3%)	38 49
1	B	247/284 (87%)	237 (96%)	10 (4%)	31 40
1	C	247/284 (87%)	241 (98%)	6 (2%)	49 62
1	D	244/284 (86%)	236 (97%)	8 (3%)	38 49
All	All	984/1136 (87%)	952 (97%)	32 (3%)	38 49

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	598	MET
1	D	622	CYS
1	B	579	ARG
1	B	573	ARG
1	D	636	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	662	ASN
1	D	597	GLN
1	D	653	ASN
1	D	631	ASN
1	B	549	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	8001	-	4,4,4	0.24	0	6,6,6	0.05	0
3	ACP	C	802	-	16,19,33	0.65	0	15,28,52	0.90	1 (6%)
2	SO4	C	801	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	A	801	-	4,4,4	0.25	0	6,6,6	0.09	0
3	ACP	D	802	-	16,19,33	0.62	0	15,28,52	0.93	1 (6%)
2	SO4	D	801	-	4,4,4	0.29	0	6,6,6	0.09	0
3	ACP	A	802	-	16,19,33	0.62	0	15,28,52	0.86	1 (6%)
3	ACP	B	8002	-	27,33,33	1.26	4 (14%)	32,52,52	1.25	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACP	A	802	-	-	0/0/17/38	0/3/3/3
3	ACP	C	802	-	-	0/0/17/38	0/3/3/3
3	ACP	B	8002	-	-	10/15/38/38	0/3/3/3
3	ACP	D	802	-	-	0/0/17/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	8002	ACP	PB-O3A	-3.87	1.54	1.58
3	B	8002	ACP	PB-O2B	-2.61	1.50	1.56
3	B	8002	ACP	PG-O2G	-2.41	1.49	1.54
3	B	8002	ACP	PG-O3G	-2.33	1.49	1.54

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	8002	ACP	O1G-PG-C3B	-3.89	102.86	111.24
3	B	8002	ACP	C5-C6-N6	2.45	124.07	120.35
3	B	8002	ACP	O2B-PB-O1B	2.34	117.87	110.07
3	A	802	ACP	C5-C6-N6	2.28	123.82	120.35
3	C	802	ACP	C5-C6-N6	2.27	123.81	120.35

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	8002	ACP	PB-C3B-PG-O1G
3	B	8002	ACP	PB-C3B-PG-O2G
3	B	8002	ACP	PB-C3B-PG-O3G
3	B	8002	ACP	PG-C3B-PB-O1B
3	B	8002	ACP	PG-C3B-PB-O3A

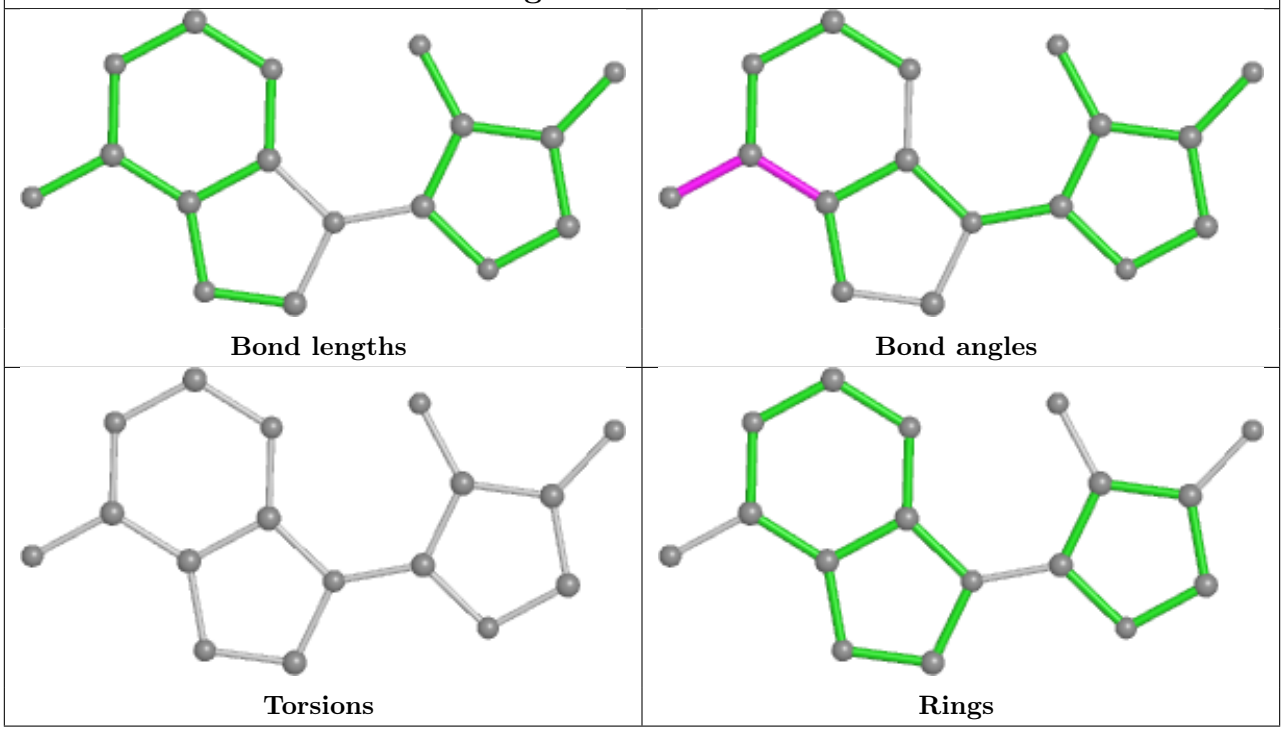
There are no ring outliers.

1 monomer is involved in 1 short contact:

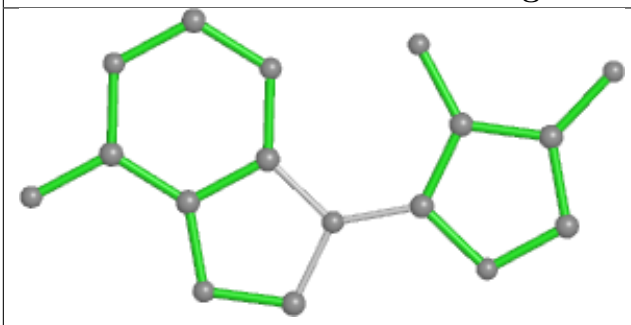
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

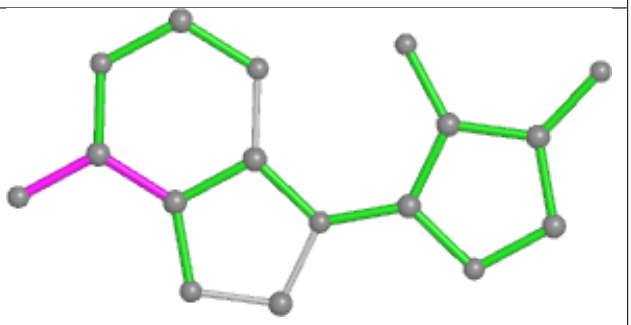
Ligand ACP C 802



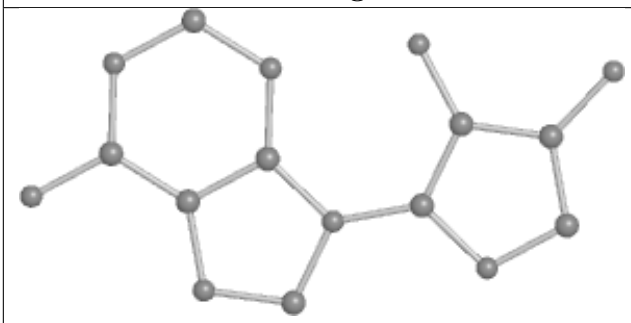
Ligand ACP D 802



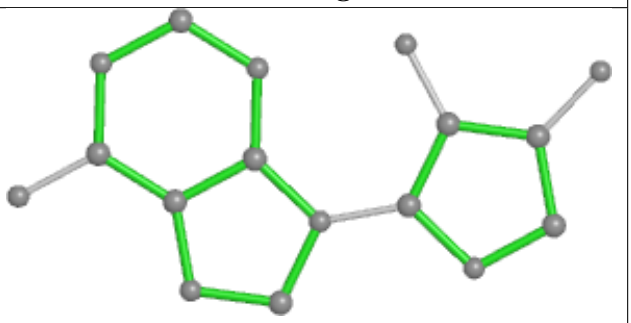
Bond lengths



Bond angles

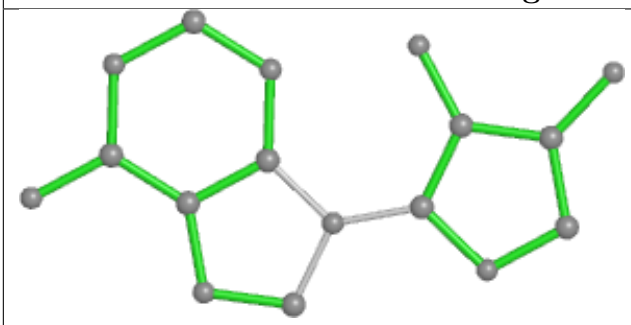


Torsions

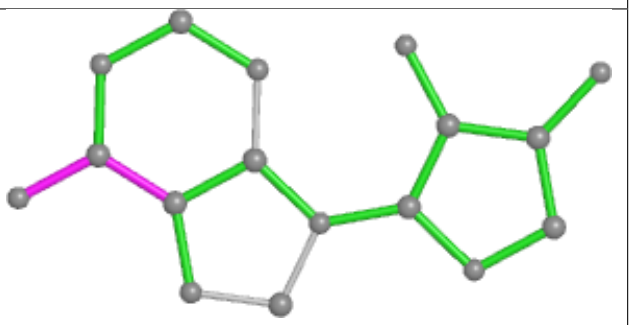


Rings

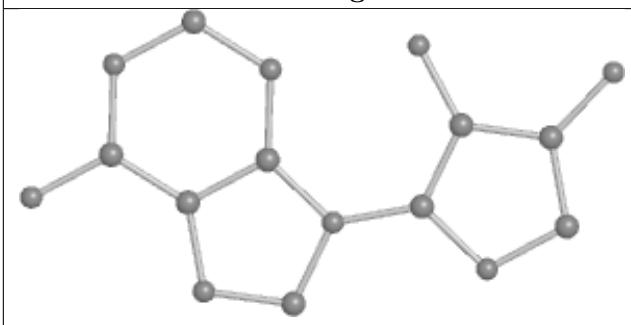
Ligand ACP A 802



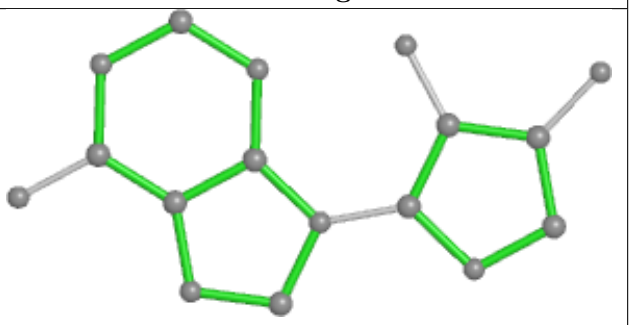
Bond lengths



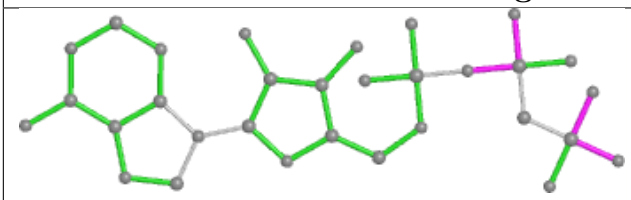
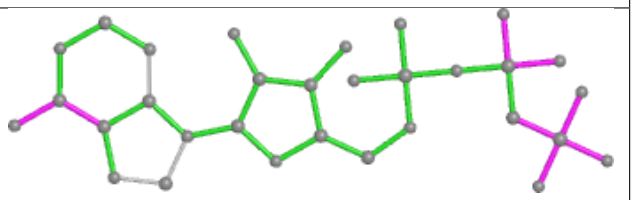
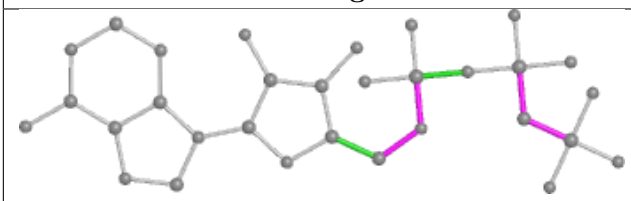
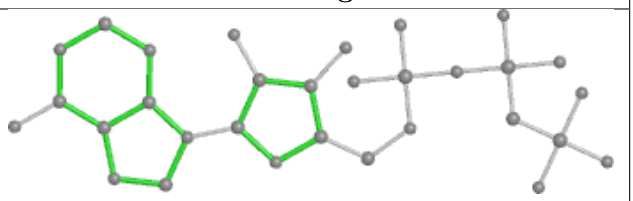
Bond angles



Torsions



Rings

Ligand ACP B 8002	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	288/324 (88%)	-0.10	6 (2%)	63	61	19, 30, 50, 61	0
1	B	286/324 (88%)	-0.01	6 (2%)	63	61	19, 34, 55, 86	0
1	C	285/324 (87%)	0.09	11 (3%)	39	37	20, 35, 59, 79	0
1	D	283/324 (87%)	-0.09	5 (1%)	68	66	16, 29, 48, 64	0
All	All	1142/1296 (88%)	-0.03	28 (2%)	57	55	16, 32, 54, 86	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	TYR	5.7
1	D	467	GLU	4.3
1	C	466	TYR	4.1
1	C	584	MET	3.7
1	B	656	TYR	3.3

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

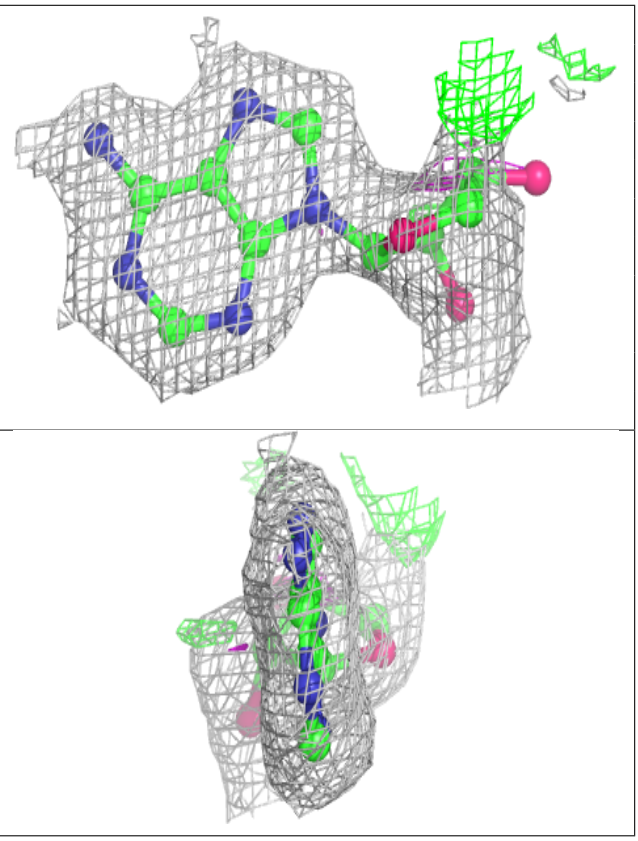
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACP	A	802	17/31	0.81	0.20	42,44,51,53	0
3	ACP	B	8002	31/31	0.85	0.19	38,58,85,85	0
3	ACP	D	802	17/31	0.88	0.16	33,39,50,54	0
2	SO4	A	801	5/5	0.89	0.17	78,79,79,79	0
3	ACP	C	802	17/31	0.91	0.14	33,36,44,46	0
2	SO4	C	801	5/5	0.95	0.16	62,62,63,63	0
2	SO4	D	801	5/5	0.95	0.12	54,54,55,55	0
2	SO4	B	8001	5/5	0.97	0.12	62,62,63,63	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

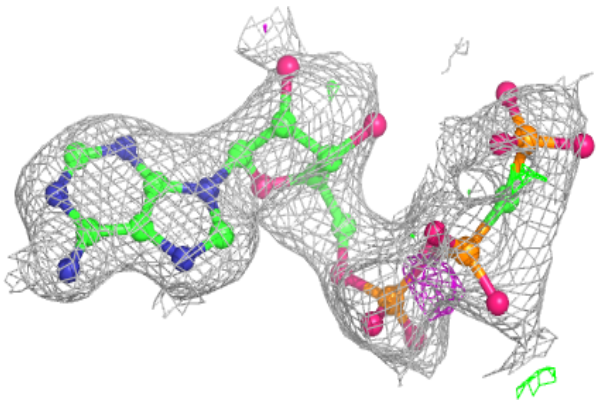
Electron density around ACP A 802:

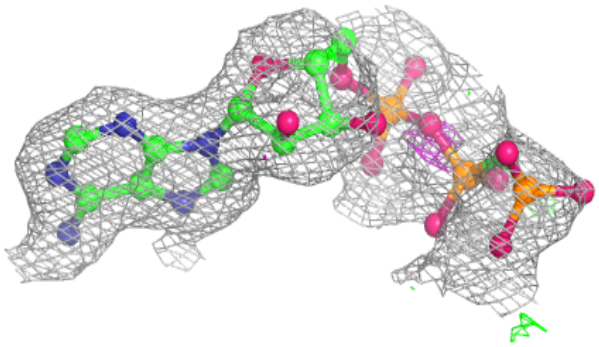
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

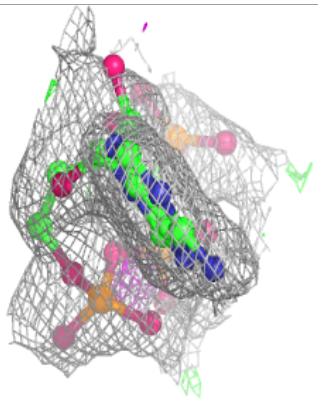


Electron density around ACP B 8002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

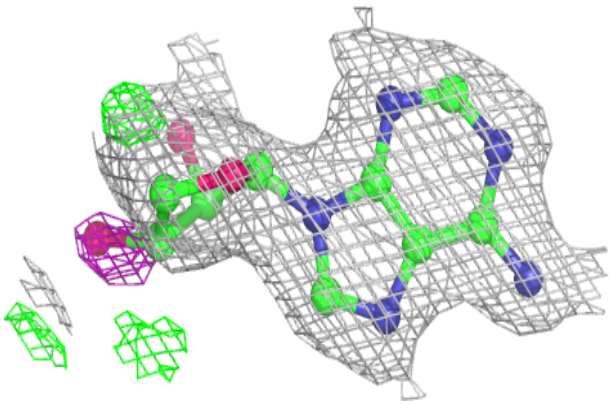


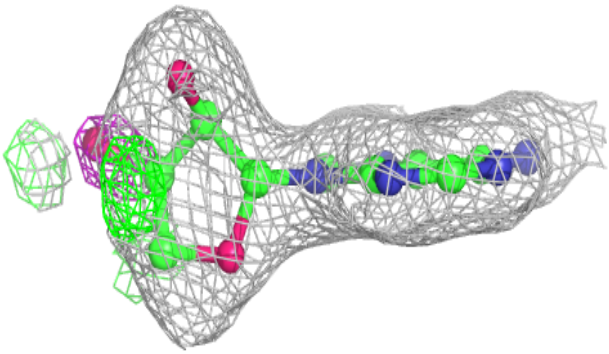


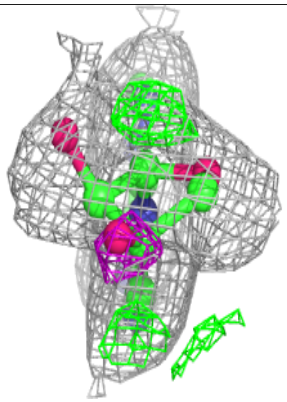


Electron density around ACP D 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

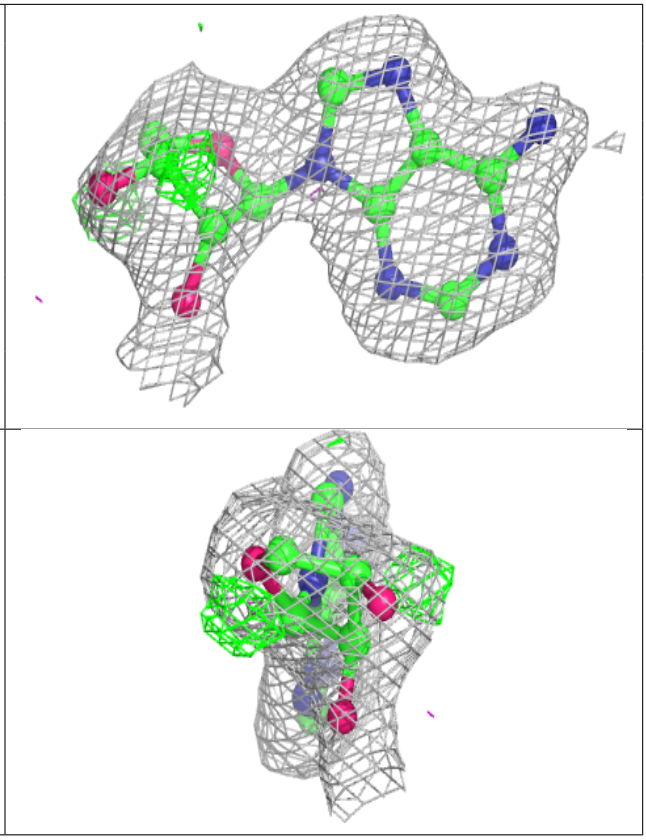






Electron density around ACP C 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.